

Optimal search strategies on complex networks

Francesca Di Patti and Duccio Fanelli

*Università degli Studi di Firenze, Dipartimento di Fisica e Astronomia and CSDC,
via G. Sansone 1, 50019 Sesto Fiorentino, Firenze, Italia and
INFN, Sezione di Firenze, Italia*

Francesco Piazza

*Université d'Orléans, Centre de Biophysique Moléculaire,
CNRS-UPR4301, Rue C. Sadron, 45071, Orléans, France*

Complex networks are ubiquitous in nature and play a role of paramount importance in many contexts. Internet and the cyberworld, which permeate our everyday life, are self-organized hierarchical graphs. Urban traffic flows on intricate road networks, which impact both transportation design and epidemic control. In the brain, neurons are cabled through heterogeneous connections, which support the propagation of electric signals. In all these cases, the true challenge is to unveil the mechanisms through which specific dynamical features are modulated by the underlying topology of the network. Here, we consider agents randomly hopping along the links of a graph, with the additional possibility of performing long-range hops to randomly chosen disconnected nodes with a given probability. We show that an optimal combination of the two jump rules exists that maximises the efficiency of target search, the optimum reflecting the topology of the network.

Let us consider a given agent (*e.g.* an electric pulse, an excitation, an animal or a human individual, such as a web surfer) located at a node of a network. The agent can hop to a neighbouring node, provided a link exists as specified by the adjacency matrix associated with the graph. The walker wanders on the network through a chain of moves, that allow for a *local* exploration of the hosting support. In such situations, the efficiency in reaching a specified location may be quantified by the mean first passage time, a robust and widely used measure of transport efficiency on networks in many contexts [3, 4], from biology [13] and ecology [7, 8, 25] to road network dynamics [12] and quantum systems [11, 23].

However, local moves are not always the best option to reach a target efficiently. For example, facilitated diffusion in the cell nucleus, a mix of one-dimensional gliding along the DNA and three-dimensional jumps to adjacent DNA strands, is believed to account for the efficiency of transcription factors in finding their binding sites [6, 19]. Analogously, inspired by the behaviour of foraging animals, it has been hypothesised that the *local* exploration of a connected territory might be complemented by intermittent relocation phases in order to optimize the searching strategy [15]. Accordingly, the animal would venture off-track through ballistic runs from time to time, thus

sampling larger portions of space. In such examples, the relative duration of the local and relocation stages may control the optimization of the dual-stage strategy [21].

Walkers on complex networks could in principle rely on similar integrated strategies, possibly tuned to the heterogeneous nature of underlying support [22]. Let us consider, for example, web surfing. Starting the exploration from an arbitrary web page, one usually proceeds by following the hyperlinks which are therein made available. This is a *local* search, which the user abandons when she opens a new tab to look for a different, potentially related topic, eventually landing into another virtual compartment which will be again probed locally for some time. On a different level, the brain displays multi-layered architectures of connections that assist the finely orchestrated spatio-temporal patterns underlying brain function [5]. One may then speculate that electric signals can be transmitted across different layers, thus realizing *de facto* long-range jumps in the overall brain connectome between single-layer connected components.

Building upon such ideas, we investigate here the conditions for optimal target searches on a generic network of N nodes. In order to quantify search efficiency on a given network, we shall compute mean first passage times [16, 18, 20], which are widely used to gauge search strategies in many contexts [1, 14, 27, 30]. To investigate the combined effect of local and long-range moves, we study a simple stochastic process which accommodates for both local diffusion and long-range relocation to disconnected sites. Let \mathbf{A} denote the $N \times N$ adjacency matrix of the network, with $A_{ij} = 1$ if i and j are physically connected by a link, and $A_{ij} = 0$ otherwise. The degree of node i is given by $k_i^A = \sum_j A_{ij}$. The probability that a particle sitting at node i jumps on any other node j is specified by the following matrix

$$T_{ij} = \alpha \frac{A_{ij}}{k_i^A} + (1 - \alpha) \frac{S_{ij}}{k_i^S} \quad (1)$$

where $S_{ij} = \{0, 1\}$ are the entries of a random symmetric sparse $N \times N$ matrix, that controls the relocation via long-range hops. The density of ones in \mathbf{S} is measured by the parameter $\delta \in [0, 1]$, so that the average number of nodes that can be reached from any node i via off-network long-range jumps is $\langle k_i^S \rangle \equiv \langle \sum_j S_{ij} \rangle = N\delta$. The parameter $\alpha \in [0, 1]$ tunes the relative strength of the two competing mechanisms, local diffusion and random

relocation. When $\alpha = 1$ the walker explores the network according to a purely local rule, while in the opposite limit, $\alpha = 0$, hopping towards disconnected sites are the only allowed moves. For $\delta = 1$, the matrix \mathbf{S} is filled with ones and \mathbf{T} becomes the known Google matrix used in the PageRank Algorithm [9, 17].

We define the search time as the time needed by a particle starting at node i to reach an absorbing trap located at node j . This satisfies the following relation (see Methods)

$$t_{i \rightarrow j} = \sum_{k=1}^{N-1} (\mathbf{Z}_j^{-1})_{ik} \quad (2)$$

where $\mathbf{Z}_j = \mathbb{I}_{N-1} - \mathbf{T}_j$. The subscript j indicates an $(N-1) \times (N-1)$ submatrix obtained by suppressing the j -th row and the j -th column, while \mathbb{I}_{N-1} denotes the identity matrix of size $N-1$. To assess the overall ability of the walker to find a target, we introduce a global parameter $\langle t \rangle$ by averaging Eq. (2) over all possible starting nodes (i) and trap locations (j), that is,

$$\langle t \rangle = \frac{1}{N(N-1)} \sum_{j \neq i} t_{i \rightarrow j} \quad (3)$$

In short, $\langle t \rangle$ quantifies the ability of the walker to search for targets at the global scale of the network. The shorter $\langle t \rangle$, the more efficient the search. The quantity α acts as a free parameter – it can be adjusted to select the optimal balance between local and long-range hops, with the aim of minimizing the global exploration time.

Fig. 1 illustrates how $\langle t \rangle$ changes as a function of the relative weight of local and long-range moves for two different classes of synthetic undirected networks, the scale-free [2, 10] and the small-world [28] networks. The curves display a clear minimum, implying the existence of an optimal value of α which minimizes the search time. Exactly the same behavior is displayed by directed networks. The location of the minimum depends on the topology of the network, which defines the backbone for local diffusion, but also on the average number of sites that can be reached through a single long-range hop, $N\delta$. Remarkably, the fewer sites are accessible through long-range jumps (*i.e.* the smaller δ), the more pronounced the optimality condition (see upper insets in Fig. 1).

When $\delta \rightarrow 1$, α_{\min} approaches (but never reaches) the limiting solution $\alpha_{\min} = 0$. In this case, the walker can virtually land on any node with just one jump (the matrix \mathbf{S} is completely filled with ones), and local diffusion contributes modestly to further reduce the average searching time. Although a minimum always exists also for $\delta = 1$ (the Google Matrix case), $\langle t \rangle_{\min}$ is very close to N , the time the walker needs to reach an isolated trap when α is exactly set to zero. Conversely, when $\delta < 1$, long-range short-cuts are only available towards a subset of nodes. This is a more plausible situation, bearing in mind the afore-mentioned applications. When surfing the web, from time to time one will abandon a given area of exploration to look for the presumed central node of a new

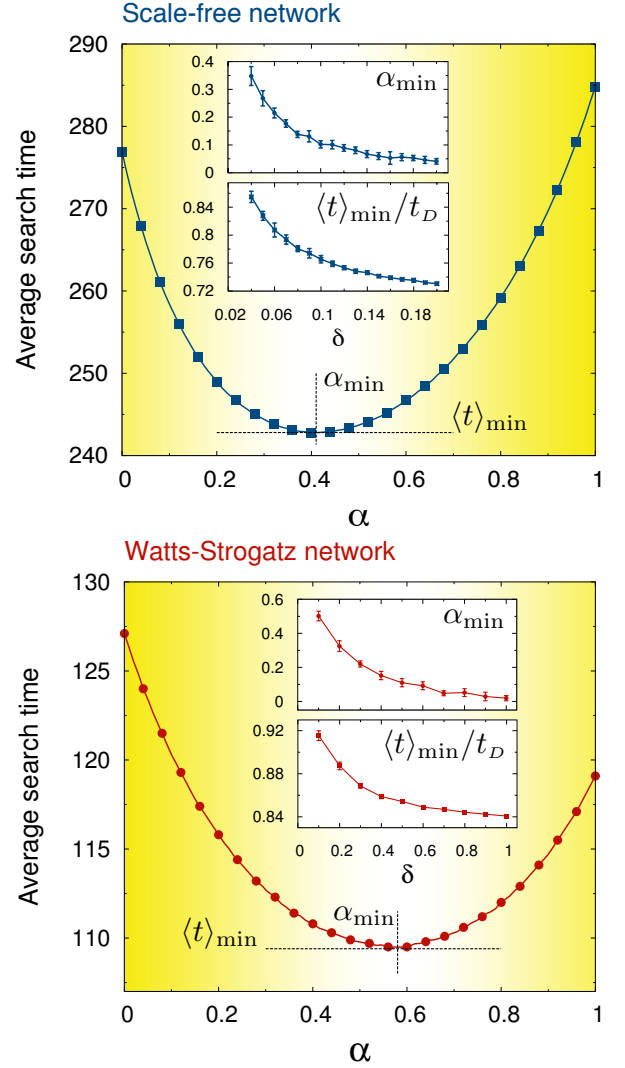


FIG. 1: **The average search time on synthetic networks displays an optimum as a function of the relative weight of local and long-range moves.** Upper panel: scale-free network generated with the preferential attachment method [2] with $N = 200$ and average connectivity $\langle k \rangle = 20$. Lower panel: Watts and Strogatz small-world random network with $p = 0.5$ [28], $N = 100$ and average connectivity $\langle k \rangle = 9.5$. Here the sparse symmetric matrix \mathbf{S} has been generated with $\delta = 0.04$ (scale-free) and $\delta = 0.1$ (Watts-Strogatz). The insets show the position of the minimum α_{\min} and the corresponding shortest average time $\langle t \rangle_{\min}$ (normalized to the case of a purely local walker, $t_D \equiv \langle t \rangle_{\alpha=1}$) as a function of the average fraction of long-range accessible nodes δ . The data are averaged over 10 independent realizations of the random matrices \mathbf{S} and error bars correspond to one standard deviation.

region that she wishes to sample. Similarly, long-range connections in the brain, established through trans-layer channels, are certainly fewer than those accounting for effective bridges among the N nodes of a given layer.

The relocation-assisted search is 10–15% more efficient with respect to the purely local dynamics for intermedi-

ate values of the density δ of available distant nodes (insets in Fig. 1). The same analysis performed with different values of the average connectivity $\langle k \rangle$ (scale-free network) and of the rewiring parameter p (Watts-Strogatz) yields similar results. In particular, upon decreasing $\langle k \rangle$ one recovers the same qualitative behaviour as obtained when increasing δ (data not shown).

To confirm the existence of an optimal searching strategy on real data sets, we have extracted the adjacency graph of small portions of the web, starting from the homepages of four main European newspapers (see Methods). The top panel of Fig. 2 shows that the general picture described above for synthetic data sets is valid for real networks too. This has nothing to do with the peculiar structure of the Web, for the same analysis performed on small neural networks of different animals confirms the existence of a clear minimum in the average search time (bottom panel in Fig. 2).

In all the cases examined, $\langle t \rangle$ appears to be a convex smooth function of α with a clear minimum. One may ask whether this is a widespread feature of many graphs. More generally, it would be helpful to have a quantitative criterion at one's disposal to predict whether an optimal search strategy exists at all, possibly also identifying the optimal balance between local and long-range moves required to place oneself in such regime. Unfortunately, the exact dependence of $\langle t \rangle$ on α is hidden in the inverse of the matrix \mathbf{Z} which, in general, cannot be computed explicitly. However, a criterion of this sort can be formulated by resorting to a perturbative approach. If we assume that the stationary point is located at sufficiently small values of α , then we may consider a search time of the form

$$\langle t \rangle \simeq c_0 - c_1\alpha + c_2\alpha^2 \quad (4)$$

In this case, the coefficients c_0 , c_1 and c_2 , which depend on the topology of the network, can be computed analytically (see Methods). A necessary and sufficient condition for a meaningful minimum to occur is $c_1 > 0$ and $c_2 > 0$ with $c_1 < 2c_2$, which ensures that $\alpha_{\min} < 1$. This provides a handy rule to enquire about the existence of an optimality condition for any given network.

In all the cases that we examined, the coefficients c_k turn out to be positive. Therefore a minimum is always predicted to exist under the quadratic approximation, and closed expressions for both α_{\min} and $\langle t \rangle_{\min}$ can be readily obtained. These match well the exact data computed through Eq. (3). The agreement is of course better when the minimum is found close to $\alpha = 0$ (Fig. 3). Explicit analytical expressions can be obtained in some limiting cases. When $\delta = 1$ one recovers the Google matrix and the transition rate from node i to node j reads $T_{ij} = \alpha A_{ij}/k_i^A + (1 - \alpha)/N$. In this case it is not difficult to show that $c_0 = N$, $c_1 = N/(N - 1)$ and $c_2 = N/(N - 1) \left[\sum_{j=1}^N \gamma_j (\gamma_j + 1/k_j^A) - N \right]$, where $\gamma_j = \sum_{i=1}^N A_{ij}/k_i^A$ (see Supplemental material for the full derivation). In the case of a regular lattice of con-

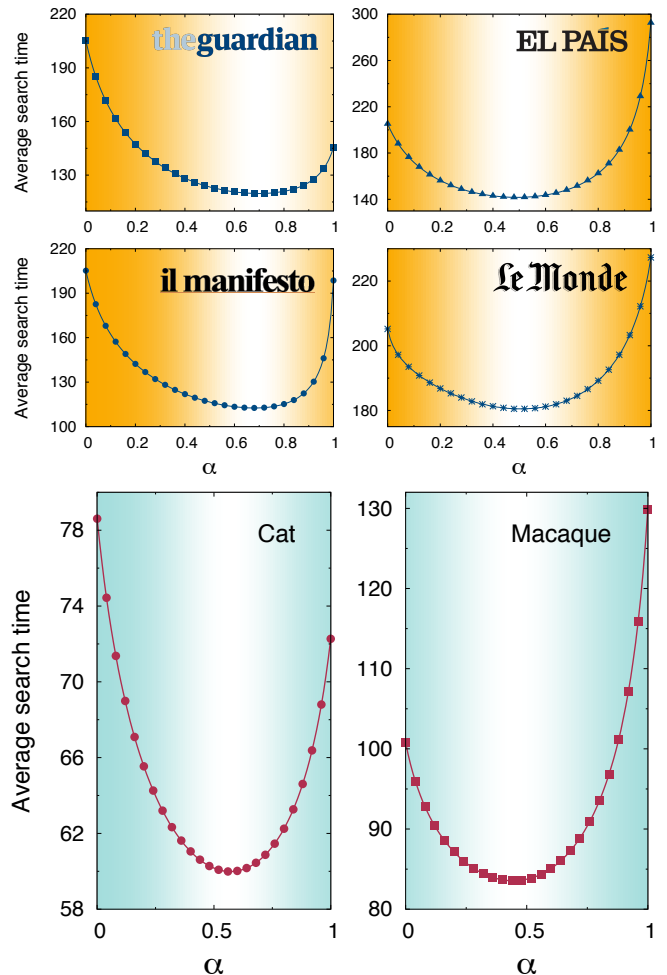


FIG. 2: The average search time on real data sets displays an optimum as a function of the relative weight of local and long-range moves. Top: average time $\langle t \rangle$ as a function of α for four real Web subgraphs. The 100×100 adjacency matrices have been mapped out by a Web crawler starting from the web sites of four major European newspapers (see Methods). The sparse symmetric matrix S has been generated with $\delta = 0.04$. Bottom: search time in two neuronal networks: cortical connectivity network of cats (52 nodes, left [24]) and macaques (71 nodes, right [29]). In both cases we have used $\delta = 0.1$.

nectivity c , one immediately finds $\alpha_{\min} = c/(2N)$ and $\langle t \rangle_{\min} = N - c/(4N)$. The more links per node are added, the larger the value of α_{\min} ($\in [1/N, 0.5]$), and the deeper the minimum for $\langle t \rangle$ vs α . Although $\langle t \rangle_{\min}$ is shorter than the search time t_D obtained for $\alpha = 0$, the associated correction is just $O(1/N)$.

Summarising, in this letter we have addressed the problem of search on networks. To this end, we have studied the trapping problem for a modified random walk, combining local hops along the links of the graph and long-range relocation jumps toward random subsets of disconnected nodes. We have shown, both for artificial and real datasets, that an optimal balance between long-

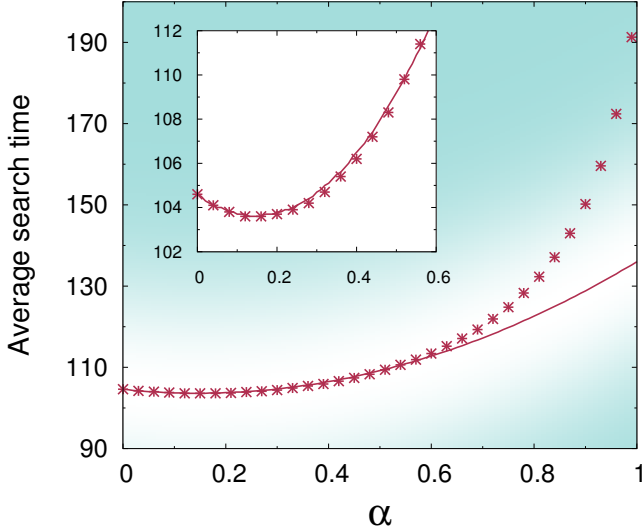


FIG. 3: **Formula (4) provides a convenient tool to enquire about the existence of an optimality criterion for the search time in a given network.** The average search time in a small random network of $N = 100$ nodes (symbols) computed from Eq. (3) is compared to the approximated quadratic profile described by Eq. (4) (solid line). The inset shows a close-up of the region around the minimum. Other parameters are: $p = 0.1$, $\delta = 0.29$.

range and local moves exists which minimizes the average time required to reach a trap. Furthermore, closed analytical expressions have been derived, enabling one to predict the optimal combination as a function of the network topology. The optimality criterion seems to be a universal dynamical mechanism, which might have exerted a critical pressure in the evolutionary selection of many naturally occurring network architectures and that might equally well be exploited in the optimization of human-made technological solutions.

Methods

Computation of first passage times. The mean first passage time t_i , namely the time it takes for a walker starting at site i to get to any one of N_Γ randomly placed traps, can be computed by extending to the case of a network the standard argument used in the continuum limit for a random walk on a line. Let us consider the interval $[0, x_0]$ on the real axis and a random walk with two absorbing boundaries located at $x = 0$ and $x = x_0$. The time interval between two jumps is Δt and the lattice spacing is Δx . The exit time $t(x)$ obeys to $t(x) = 1/2 [t(x + \Delta x) + \Delta t] + 1/2 [t(x - \Delta x) + \Delta t]$ meaning that the walker can be regarded as starting one step in the future with equal probability from either $x + \Delta x$ or $x - \Delta x$. The generalization of this equa-

tion for a random walk on a network is simply given by $t_i = \sum_j T_{ij} [t_j + \Delta t]$, a formulation which proves particularly convenient to investigate the trapping problem. Indeed, re-labelling the nodes of the network so as to have non-trap nodes going from 1 to $N - N_\Gamma$ and all traps located at nodes $N - N_\Gamma + 1$ to N , one obtains a matrix \mathbf{T} with the last N_Γ rows equal to zero. Rearranging correspondingly the array t_i and recalling that $t_i = 0$ for $N - N_\Gamma + 1 \leq i \leq N$, one finds that the exit times are solution of the linear system $\sum_{j=1}^{N-N_\Gamma} Z_{ij} t_j = 1$, where we have denoted by \mathbf{Z} the upper-left $(N - N_\Gamma) \times (N - N_\Gamma)$ block square sub-matrix of $\mathbf{T} - \mathbb{I}_N$. Eq. (2) is the formal solution of this last equation.

Adjacency matrices of sub-networks from the web. To gather real data from the Web we have used the Web crawler *surfer.m* (<http://www.mathworks.com/>). Starting from a selected URL, the crawler identifies all the hyperlinks in the page and adds them to the list of URLs to visit. Once all these URLs are visited, the procedure is repeated recursively for each URL in the list until the assigned number of websites is reached. The outcome of the algorithm is stored in an adjacency matrix where nodes represent the visited pages: the entries of the matrix are 1 if two pages are connected through a hyperlink, 0 otherwise. The matrix is then symmetrized.

Perturbative expansion of a sum of two matrices. Let \mathbf{C} and \mathbf{B} be two arbitrary non-singular square matrices of the same dimension and let us introduce the operator Θ , that returns the sum of all the elements of a given square matrix. Starting from the relation $(\mathbf{C} + \epsilon \mathbf{B})^{-1} = (\mathbb{I}_N + \epsilon \mathbf{C}^{-1} \mathbf{B})^{-1} \mathbf{C}^{-1}$, and expressing $\epsilon \mathbf{C}^{-1} \mathbf{B}$ by a Neumann series [26], it follows $(\mathbf{C} + \epsilon \mathbf{B})^{-1} = \mathbf{C}^{-1} - \epsilon \mathbf{C}^{-1} \mathbf{B} \mathbf{C}^{-1} + \epsilon^2 \mathbf{C}^{-1} \mathbf{B} \mathbf{C}^{-1} \mathbf{B} \mathbf{C}^{-1} + \dots$. To apply this approximation to Eq. (3), we introduce two diagonal matrices associated with \mathbf{A} and \mathbf{S} , namely $\mathbf{K}_\mathbf{A} = \text{diag}(k_1^A, \dots, k_N^A)$ and $\mathbf{K}_\mathbf{S} = \text{diag}(k_1^S, \dots, k_N^S)$. In this way, \mathbf{T} takes the form $\alpha \mathbf{K}_\mathbf{A}^{-1} \mathbf{A} + (1 - \alpha) \mathbf{K}_\mathbf{S}^{-1} \mathbf{S}$. Consequently, by denoting again by j the position of the trap, the terms of the reduced matrix \mathbf{Z}_j can be easily rearranged by collecting together those proportional to α . In formulae: $\mathbf{Z}_j = \mathbb{I}_{N-1} - (\mathbf{K}_\mathbf{S}^{-1})_j \mathbf{S}_j + \alpha [(\mathbf{K}_\mathbf{S}^{-1})_j \mathbf{S}_j - (\mathbf{K}_\mathbf{A}^{-1})_j \mathbf{A}_j]$. Setting $\mathbf{C}_j = \mathbb{I}_{N-1} - (\mathbf{K}_\mathbf{S}^{-1})_j \mathbf{S}_j$, $\mathbf{B}_j = (\mathbf{K}_\mathbf{S}^{-1})_j \mathbf{S}_j - (\mathbf{K}_\mathbf{A}^{-1})_j \mathbf{A}_j$ and $\epsilon = \alpha$, and applying the operator $\Theta(\cdot)$ to $(\mathbf{C}_j + \epsilon \mathbf{B}_j)^{-1}$, we recover Eq. (4) with $c_0 = \sum_j \Theta(\mathbf{C}_j^{-1}) / N / (N - 1)$, $c_1 = \sum_j \Theta(\mathbf{C}_j^{-1} \mathbf{B}_j \mathbf{C}_j^{-1}) / N / (N - 1)$ and $c_2 = \sum_j \Theta(\mathbf{C}_j^{-1} \mathbf{B}_j \mathbf{C}_j^{-1} \mathbf{B}_j \mathbf{C}_j^{-1}) / N / (N - 1)$.

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